

CLAIMS

What is claimed is:

1. A method of data processing and evaluation comprising the steps of:
 - (a) correcting the data points of a chromatogram for baseline to provide a corrected-chromatogram;
 - (b) smoothing the data points of the chromatogram to provide a smoothed-corrected-chromatogram; and
 - (c) determining an entropy value for the smoothed-corrected-chromatogram based on the product of a data point value and a logarithm of the data point value for a plurality of data points of the smoothed-corrected-chromatogram.

2. The method of claim 1, wherein the entropy value of a smoothed-corrected-chromatogram is defined substantially by

$$H = \sum_{i=1}^n p_i \ln(p_i),$$

where H is the entropy value, and p_i is the intensity value of the i^{th} data point of the smoothed-corrected-chromatogram.

3. The method of claim 2, further comprising the steps of:
 - repeating steps (a) to (c) for a plurality of chromatograms of a data set; and
 - determining a quality factor for a smoothed-corrected-chromatogram based on the entropy values of the plurality of chromatograms of the data set, the quality factor defined substantially by

$$IQ = 1 - (H/H_{\max}),$$

where IQ is the quality factor, H is the entropy value of the smoothed-corrected-chromatogram, and H_{\max} is the maximum entropy value of the plurality of chromatograms of the data set.

4. The method of claim 3 further comprising the step of generating a reconstructed total ion current chromatogram from a plurality of smoothed-corrected-

chromatograms selected based on the quality factor of the individual smoothed-corrected-chromatograms.

5. The method of claim 4 further comprising the step of:

assigning a mass signal quality value to each of one or more mass signals based on the difference between data points values corresponding to a mass signal before steps (a) and (b) and data points values corresponding to a mass signal after steps (a) and (b),

wherein the step of generating a reconstructed total ion current chromatogram comprises excluding from the reconstructed total ion current chromatogram one or more mass signals selected based on the mass signal quality value of the individual mass signals.

6. The method of claim 1, further comprising the step of assigning a mass signal quality value to each of one or more mass signals based on the difference between data points values corresponding to a mass signal before steps (a) and (b) and data points values corresponding to a mass signal after steps (a) and (b).

7. The method of claim 6, further comprising the step of determining a correlation between each of a plurality of chromatograms of a data set and a smoothed-corrected-chromatogram associated with one or more mass signals selected based on the mass signal quality value of the individual mass signals.

8. The method of claim 7 wherein the step of determining a correlation comprises performing a multivariate analysis of the chromatograms of the data set with respect to the smoothed-corrected-chromatogram associated with one or more mass signals selected based on the mass signal quality value of the individual mass signals.

9. The method of claim 1 wherein the step of smoothing comprises use of a methodology substantially defined by a Savitsky-Golay algorithm.

10. A method of data processing and evaluation comprising the steps of:

(a) correcting the data points of a chromatogram for baseline to provide a corrected-chromatogram;

(b) smoothing the data points of the chromatogram to provide a smoothed-corrected-chromatogram; and

(c) determining an entropy value for the smoothed-corrected-chromatogram based on the product of a data point value and a logarithm of the data point value for a plurality of data points of the smoothed-corrected-chromatogram;

(d) repeating steps (a) to (c) for a plurality of chromatograms of a data set;

(e) determining a quality factor for a smoothed-corrected-chromatogram based on the entropy values of a plurality of chromatograms of the data set;

(f) assigning a mass signal quality value to each of one or more mass signals based on the difference between data points values corresponding to a mass signal before steps (a) and (b) and data points values corresponding to a mass signal after steps (a) and (b);

(g) determining a correlation between each of a plurality of chromatograms of a data set and a smoothed-corrected-chromatogram associated with one or more mass signals selected based on the mass signal quality value of the individual mass signals.

11. The method of claim 10 wherein the step of determining a correlation comprises performing a multivariate analysis of the chromatograms of the data set with respect to the smoothed-corrected-chromatogram associated with one or more mass signals selected based on the mass signal quality value of the individual mass signals.

12. An article of manufacture having computer-readable program means for performing the method of claim 10 embodied thereon.

13. A system for data processing and evaluation comprising:
a baseline correction device;
a smoothing device for smoothing the data points of a chromatogram,

an entropy value device for determining an entropy value for the chromatogram based on the product of the value of a data point and a logarithm of the data point value for a plurality of data points of the chromatogram; and a selection device for selecting chromatograms based on their entropy values.

14. The system of claim 13 further comprising a summing device for generating a reconstructed total ion current chromatogram based on chromatograms selected by the selection device.

15. The system of claim 14 wherein the selection device is further adapted to select one or more mass signals and the summing device is adapted to exclude from the reconstructed total ion current chromatogram the one or more selected mass signals.

16. The system of claim 13 further comprising a correlator for determining a correlation between a plurality of chromatograms of a data set and a chromatogram associated with one or more selected mass signals.

17. The system of claim 16 wherein the correlator comprises a multivariate analyzer for performing a multivariate analysis of at least one of a selected chromatogram and one or more selected mass signals with respect to a plurality of chromatograms of a data set.